

# PhD student position (m/f/d) - Computational Materials Science/ Theoretical/Computational Chemistry/Physics

Start of announcement 15.10.2019

End of announcement 12.11.2019

Institute Institute of Materials Research

Location Geesthacht (near Hamburg)

The Institute of Materials Research of **Helmholtz-Zentrum Geesthacht** is offering a **PhD student position (m/f/d) in multiscale modeling of hydrogen storage materials**. The position is initially limited for three years (starting as soon as possible). The place of employment is Geesthacht.

In the framework of our research on “Novel Complex Metal Hydrides for Efficient and Compact Hydrogen Storage” the Institute of Materials Research at HZG is offering a positions for a post graduate student interested in the **development and simulation of hydrides and hydride composites for solid state hydrogen storage**. The aim of this work is the characterization, understanding and optimization of novel complex and light metal hydrides as well as their composites for hydrogen storage and batteries. The results are the basis for further optimisation of such materials for mobile and stationary energy storage applications.

The project will be conducted as part of a young, multidisciplinary and highly motivated team within the newly established **division for Computation and Simulation**. The goal is to form close connections between the team members to approach problems from different perspectives and to create an atmosphere where creative ideas and exchange of knowledge can thrive. Furthermore, the project will be part of a close **collaboration with a renown research institute in the USA** which will involve frequent research stays at the partner institution.

## Tasks:

- the position involves primarily the **simulation of the kinetic properties of complex and metal hydrides by means of Phase Field simulations**. This will involve running and modifying the deployed code and thorough scientific interpretation of the calculated data. At a later stage, First-Principles Molecular Dynamics Simulations might also become part of the methodology
- **collaboration** with experimental partners at HZG and the US partner institution
- the candidate is expected to present the results on project meetings, international conferences, and in scientific publications and to contribute to patent applications

## We are looking for:

- curiosity-driven, highly motivated and detail-oriented personality who integrates well into an interdisciplinary team
- self-dependent and pro-active attitude
- excellent problem solving skills, creative thinking and the ability to quickly learn new methods and techniques

## Qualifications:

- a **master's degree in computational materials science, theoretical/computational chemistry, physics, inorganic chemistry** (or related fields) is required
- experiences in the area of **Phase Field simulations** for kinetic and thermodynamic properties of hydrides or metallic alloys are highly desired
- expertise with **quantum chemical methodology (DFT, ab-initio), Molecular Dynamics, Monte Carlo** are beneficial
- **strong mathematical background and programming experience** are essential
- knowledge in metal hydrides and/or hydrogen technology would be an additional advantage
- **very good English speaking and writing skills** as well as presentation/communication skills are expected
- **ability to travel** as necessary (up to several months per year)

## For further information please contact:

[Dr. Paul Jerabek \(paul.jerabek@hzg.de\)](mailto:paul.jerabek@hzg.de)

## We offer you:

- multinational work environment with over 950 colleagues from more than 50 nations
- extensive options of vocational training (i. a. expert seminars, language courses or leadership seminars)
- flexible working hours and various models to ensure ensure the compatibility of family and career
- excellent infrastructure including modern work spaces
- remuneration according to the standards of the collective wage agreement TV-AVH including further social benefits

The promotion of equal rights is a matter of course for us. Severely disabled persons and these equals disable peoples equally suitable for a position will be given preference in accordance with statutory provisions.

Interested? Then we are looking forward to receiving your comprehensive application documents (CV, copies of degrees and other qualifications, research interests, publication list) indicating the reference number **code no. 2019/WT 5**

Please start the online application process for this offered position here:

[https://www.hzg.de/campus\\_career/vacencies/016301/index.php.en](https://www.hzg.de/campus_career/vacencies/016301/index.php.en)

**Closing date for applications is November 12th, 2019.**